An improved effective field theory formulation of spin-1/2 Ising systems with arbitrary coordination number z

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1 Abstract

An improved unified formulation based on the effective field theory is introduced for a spin-1/2 Ising model with nearest neighbor interactions with arbitrary coordination number z. Present formulation is capable of calculating all the multi-spin correlations systematically in a representative manner , as well as its single site counterparts in the system and gives results for the critical temperature of the system much better than those of the other works in the literature. The formulation can be easily applied to various extensions of s-1/2 Ising models, as long as the system contains only the nearest neighbor interactions as spin-spin interactions. Keywords: **Ising model ; Effective field theory ;Correlation functions**

2 Introduction

Ising model [1] has been one of the most extensively studied models in statistical mechanics and condensed matter physics for a long time. The reason is due to the fact that this simple many-body system suits well for investigation of thermal and magnetic properties of various physical systems. From the theoretical point of view, this model has been handled by a variety of approximation techniques and each of them were developed for a demand of obtaining better results, especially for determination of critical temperature of the system as accurate as the known exact results. Bethe-Peierls approximation (BPA) [2], Bethe lattice approximation (BLA) [3] the effective field theory (EFT) [4] the correlated effective field theory (CEFT) [5] the cluster variation method (CVM) [6] the series expansion methods (SE) [7] and expanded Bethe-Peierls approximation (EBPA) [8] are among the most widely used approximations for the s-1/2 Ising systems. Among these methods, EFT in which the system is treated as a finite cluster is regarded as one of the most powerful methods which gives rather accurate results than those of conventional mean field theory which considers a many-body system as a single particle system.

In a typical EFT method [9] , one writes the spin interactions on a finite cluster explicitly by choosing an appropriate Hamiltonian. Contributions coming from the outside of the defined cluster are represented by an effective field, and determination of this effective field plays a key role for solving the problem. Another alternative choice is to work on a larger cluster and to define the interactions only within this larger finite cluster [10],[11]. In EFT methods, calculations are often carried on by starting with exact spin identities [12],[13]. These identities include the thermal average of some certain functions which depend on the spin variables in the cluster. Hence, in addition to the single spin cluster identities there are several works based on two or more spin cluster identities in the literature [10],[11]. Whatever form of identities used, in order to perform the thermal averages, differential operator [4] and integral operator techniques [14],[15] are often used. However, the accuracy and responsibility of the results obtained by these EFT methods costs some complicated mathematical difficulties. Namely, it is widely believed that if one tries to treat exactly all the spin-spin correlations emerging on the expansion of the spin identities then the problem becomes mathematically intractable. In order to overcome these difficulties, one often has to make an approximation on the problem of evaluating the correlation functions which means a less accuracy of the results in comparison with the exact ones. Hence, it is no matter that whatever the technique is used, the most of the studies in the literature refer to a decoupling approximation (DA) which neglects the multi-spin correlations [4] and gives the results identical to those of Zernike approximation [16]. However there are small number of works try to handle these correlations [5],[9]. Although they have different formulations, these two works gives results which are identical to those of BPA for the critical temperatures.

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Recently, we have introduced an improved formulation, based on differential operator technique for investigation of the thermal and magnetic properties of a 3D random field Ising model [17]. Our formulation improves the results of the conventional EFT methods by taking into account the multi-spin correlations. In this paper, we wish to extend the method given in Ref. [17] for a general Ising s-1/2 system with nearest neighbor interactions by proposing a unified formulation which systematically includes the multi-spin correlation effects for a given arbitrary coordination number z. The general formulation being presented here can be easily adopted to more complicated systems such as the models with transverse field. For this purpose, we organized the paper as follows: In Sec. 3 we explicitly present the formulations. The numerical results and discussions are summarized in Sec. 4 with application of formulation to pure system and bond diluted system and finally Sec. 5 contains our conclusions.

3   General formulation

The Hamiltonian describing our model is

$$\mathcal{H} = -\sum_{<i,j>} J_{ij} s_i s_j - \sum_i H_i s_i \tag{1}$$

Here s_i denotes the z component of the spin variable and it takes the values $s_i = \pm 1$, $J_{ij} = J_{ji} > 0$ is the ferromagnetic exchange interaction between spins i and j, and H_i is the external longitudinal magnetic field on a site i. The first summation in Eq. (1) is over the nearest-neighbor pairs of spins and the other summation is over the all lattice sites. The quantities J_{ij}, and H_i may be given with certain distributions or they can have the same values for all pairs of spins/sites, i.e $J_{ij} = J, H_i = H$.

As our model system, we consider a regular lattice which has N identical spins arranged with coordination number z. We define a cluster on the lattice which consists of a central spin labeled s_0, and z perimeter spins ($s_\delta, \delta = 1, 2, \ldots z$) being the nearest-neighbors of the central spin. The nearest-neighbor spins are in an effective field produced by the outer spins, which can be determined by the condition that the thermal and configurational average of the central spin is equal to that of its nearest-neighbor spins.

According to the Callen identity [12], averages of the spin variables in the cluster are given by

$$\langle\langle\{f_i\}s_i\rangle\rangle_r = \langle\langle\{f_i\}\tanh(\beta E_i)\rangle\rangle_r \tag{2}$$

where $\beta = 1/k_B T$, k_B is Boltzmann constant and T is the temperature, E_i is the part of the Hamiltonian in Eq. (1) which includes all contributions associated with the site i and $\{f_i\}$ is an arbitrary function which is independent of the site i. The inner average bracket (which has no subscript) stands for thermal average and the outer one (which has subscript r) is for configurational average which is necessary for including the effect of random bond and random field distributions.

At this stage, Eq. (2) is exact but it is not possible to perform the averages without making an approximation due to the large number of degrees of freedom of the system. One coarse approximation is well known mean field approximation. In this approximation (for the system homogenous distributed bonds, i.e. $J_{ij} = J$ for all i, j and zero magnetic field) the spin s_i interacts with the field $Jz\langle s\rangle$ where $\langle s\rangle = \langle s_i\rangle, i = 0, 1, \ldots, z$. Thus, in this approximation magnetization is given by

$$\langle s\rangle = \tanh(\beta J z \langle s\rangle) \tag{3}$$

On the other hand within the EFT, average of the central spin is obtained from Eq. (2) with $E_0 = -\sum_{\delta=1}^z J_{0\delta} s_\delta - H_0$ as

$$\langle\langle\{f_0\}s_0\rangle\rangle_r = \left\langle\left\langle\{f_0\}\tanh\left(\beta\sum_{\delta=1}^z J_{0\delta} s_\delta + \beta H_0\right)\right\rangle\right\rangle_r. \tag{4}$$

By choosing $\{f_0\} = 1$, we can get the thermal and configurational average of a central spin from Eq. (4). In a similar manner, perimeter spin in the cluster, interacts with central spin and with an

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effective field which is produced by the $(z-1)$ spins outside of the cluster. Hence, the average of the perimeter spin can be obtained again from Eq. (2), but this time with $E_\delta = -J_{0\delta}s_0 - (z-1)h - H_\delta$.

$$\langle\langle\{f_\delta\}s_\delta\rangle\rangle_r = \langle\langle\{f_\delta\}\tanh\left(\beta J_{0\delta}s_0 + \beta(z-1)h + \beta H_\delta\right)\rangle\rangle_r \tag{5}$$

where h is the effective field per spin. By choosing $\{f_\delta\} = 1$, we get the average of the perimeter spin from Eq. (5) . Since all the sites are equivalent in the model, the value of the effective field h for a fixed temperature and certain distributions can be determined from the relation

$$\langle\langle s_0\rangle\rangle_r = \langle\langle s_\delta\rangle\rangle_r \tag{6}$$

Hence, for a given (β, h) pair with a certain bond and longitudinal magnetic field distribution, we can obtain magnetization as a function of the temperature. Since the effective field is very small in the vicinity of critical temperature then the critical temperature can be obtained by letting $h \to 0$ in Eq. (6) and solving it for $\beta = \beta_c$ where $\beta_c = 1/k_B T_c$, T_c is the critical temperature.

In order to evaluate right hand sides of Eqs. (4) and (5) we can apply the differential operator technique [4]

$$\exp(a\nabla)f(x) = f(x+a) \tag{7}$$

where $\nabla = \partial/\partial x$ is the differential operator and a is any constant. With the help of Eq. (7) we get the following equations

$$\langle\langle\{f_0\}s_0\rangle\rangle_r = \left\langle\left\langle\{f_0\}\prod_{\delta=1}^{z}\left[\cosh(J_{0\delta}\nabla) + s_\delta \sinh(J_{0\delta}\nabla)\right]\right\rangle\right\rangle_r f(x)|_{x=0} \tag{8}$$

$$\langle\langle\{f_\delta\}s_\delta\rangle\rangle_r = \langle\langle\{f_\delta\}\left[\cosh(J_{0\delta}\nabla) + s_0 \sinh(J_{0\delta}\nabla)\right]\rangle\rangle_r f(x+(z-1)h)|_{x=0} \tag{9}$$

where

$$f(x) = \int dH_i P_H(H_i)g(x, H_i), \quad g(x, H_i) = \tanh[\beta(x+H_i)]. \tag{10}$$

Here $P_H(H_i)$ is the probability distribution function of longitudinal magnetic field.

By expanding the right hand side of Eq. (8) with $\{f_0\} = 1$ we can obtain the thermal and configurational average of the central spin. This expansion which is superior to conventional MFA takes into account the self-spin correlation identity which is given by

$$s_i^{2n} = 1, s_i^{2n-1} = s_i \tag{11}$$

for all i where n is positive integer and the expansion produces the multi-spin correlations among the perimeter spins for s-1/2 Ising system. In order to avoid dealing with the mathematical difficulties originating from these multi-spin correlations, an approximation which is widely used in the literature, i.e. DA [18] can be used according to

$$\langle\langle s_i s_j \dots s_k\rangle\rangle_r = \langle\langle s_i\rangle\rangle_r \langle\langle s_j\rangle\rangle_r \dots \langle\langle s_k\rangle\rangle_r. \tag{12}$$

However, the multi-spin correlations can be evaluated by using an appropriate $\{f_\delta\}$ variable and expanding Eq. (9). In other words, we can calculate any correlation which includes only perimeter spins from Eq. (9) by using an appropriate $\{f_\delta\}$. Moreover, if we expand the right hand side of Eq. (9) with a selected $\{f_\delta\}$ some other correlations appear which are represented in terms of the central spin and perimeter spins in the cluster. Similarly, these correlations can also be calculated by using Eq. (8) and by selecting a suitable $\{f_0\}$. As a result of this process, we obtain a set of linear equations in which all correlations are treated as unknowns. Since this approximation takes into account the multi-spin correlations, it gives better results than those obtained by EFT with DA.

Now, in order to obtain a system of linear equations with arbitrary coordination number z, let us write Eq. (8) as,

$$\langle\langle\{f_0\}s_0\rangle\rangle_r = \left\langle\left\langle\{f_0\}\sum_{n=0}^{z}\left[\binom{z}{n}\prod_{\delta=1}^{n}s_\delta\sinh(J_{0\delta}\nabla)\prod_{\delta=n+1}^{z}\cosh(J_{0\delta}\nabla)\right]\right\rangle\right\rangle_r f(x)|_{x=0} \tag{13}$$

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While writing Eq. (8) as Eq. (13) we use an approximation that all n multi-site correlations among the perimeter spins are equal to each other and we represent them with $\left\langle\left\langle s_\delta^{(n)} \right\rangle\right\rangle_r = \left\langle\langle s_1 s_2 \ldots s_n\rangle\right\rangle_r$. In other words we represent $\begin{pmatrix} z \\ n \end{pmatrix}$ possible n-site perimeter spin correlations with one correlation. For example for $z = 3, n = 2$, the correlations

$$\langle\langle s_1 s_2\rangle\rangle_r = \langle\langle s_2 s_3\rangle\rangle_r = \langle\langle s_1 s_3\rangle\rangle_r$$

are identical and represented as $s_\delta^{(2)} = s_1 s_2$. The same approximation holds also for multi-site correlations which include central site s_0 i.e. $\left\langle\left\langle s_0 s_\delta^{(n-1)} \right\rangle\right\rangle_r = \langle\langle s_0 s_1 \ldots s_{n-1}\rangle\rangle_r$ represents all n-site correlations which include the central site.

Now, since all the terms except s_δ are independent of the thermal average then we can write Eq. (13) in the form:

$$\langle\langle\{f_0\} s_0\rangle\rangle_r = \sum_{n=0}^{z} A_n \left\langle\left\langle \{f_0\} s_\delta^{(n)} \right\rangle\right\rangle_r \tag{14}$$

where $s_\delta^{(n)} = s_1 s_2 \ldots s_n$ and the coefficient A_n is given by

$$A_n = \begin{pmatrix} z \\ n \end{pmatrix} \left\langle \left[\prod_{\delta=1}^{n} \sinh\left(J_{0\delta}\nabla\right) \prod_{\delta=n+1}^{z} \cosh\left(J_{0\delta}\nabla\right) \right] \right\rangle_r f(x)|_{x=0} \tag{15}$$

The configurational average can be taken by using any given bond distribution probability function $P_J\left(J_{ij}\right)$

$$A_n = \begin{pmatrix} z \\ n \end{pmatrix} \left[\int \prod_{\delta=1}^{z} [dJ_{0\delta} P_J\left(J_{0\delta}\right)] \prod_{\delta=1}^{n} [\sinh\left(J_{0\delta}\nabla\right)] \prod_{\delta=n+1}^{z} [\cosh\left(J_{0\delta}\nabla\right)] \right] f(x)|_{x=0} \tag{16}$$

The derivation of the multi-site correlations by adopting a suitable $\{f_0\}$ in Eq. (14) requires the determination of the identity $\left\langle\left\langle \{f_0\} s_\delta^{(n)} \right\rangle\right\rangle_r$ which lies on the right-hand side of Eq. (14). Let us call choosing $\{f_0\} = s_k$ in this term as applying s_k to $\left\langle\left\langle s_\delta^{(n)} \right\rangle\right\rangle_r$. Applying s_k to $\left\langle\left\langle s_\delta^{(n)} \right\rangle\right\rangle_r$ will yield another correlation. Resulting correlation may be $\left\langle\left\langle s_\delta^{(n-1)} \right\rangle\right\rangle_r$ or $\left\langle\left\langle s_\delta^{(n+1)} \right\rangle\right\rangle_r$ depending on the relation between k and n. For determining the resulting correlation we use Eq. (11) and it will be given by

$$\left\langle\left\langle s_k s_\delta^{(n)} \right\rangle\right\rangle_r = \begin{cases} \left\langle\left\langle s_\delta^{(n+1)} \right\rangle\right\rangle_r &, \quad k > n \\ \left\langle\left\langle s_\delta^{(n-1)} \right\rangle\right\rangle_r &, \quad k \leq n \end{cases} \tag{17}$$

According to Eq. (17), if we select $\{f_0\} = s_1$ in Eq. (14) then we get

$$\langle\langle s_0 s_1\rangle\rangle_r = A_1 + (A_0 + A_2) \langle\langle s_1\rangle\rangle_r + \sum_{n=3}^{z} A_n \left\langle\left\langle s_\delta^{(n-1)} \right\rangle\right\rangle_r \tag{18}$$

Similarly, if we apply s_2 to Eq. (18) we obtain

$$\langle\langle s_0 s_1 s_2\rangle\rangle_r = (A_1 + A_3) \langle\langle s_1\rangle\rangle_r + (A_0 + A_2 + A_4) \langle\langle s_1 s_2\rangle\rangle_r + \sum_{n=5}^{z} A_n \left\langle\left\langle s_\delta^{(n-2)} \right\rangle\right\rangle_r \tag{19}$$

After successive operations, we can get a general expression for the correlation $\langle\langle s_0 s_1 s_2 \ldots s_k\rangle\rangle_r$ as follows

$$\left\langle\left\langle s_0 s_\delta^{(k)} \right\rangle\right\rangle_r = \left\langle\left\langle s_\delta^{(k-1)} \right\rangle\right\rangle_r \sum_{n=0}^{k-1} A_{2n+1} + \left\langle\left\langle s_\delta^{(k)} \right\rangle\right\rangle_r \sum_{n=0}^{k} A_{2n} + \sum_{n=2k+1}^{z} A_n \left\langle\left\langle s_\delta^{(n-k)} \right\rangle\right\rangle_r \tag{20}$$

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Multi-site correlations which appear on the right hand side of Eq. (20) can be obtained from Eq. (9). Writing Eq. (9) for $\delta = 1$ and choosing $\{f_1\} = s_2$ in this expression will yield

$$\langle\langle s_1 s_2 \rangle\rangle_r = B_1 \langle\langle s_1 \rangle\rangle_r + B_2 \langle\langle s_0 s_1 \rangle\rangle_r \tag{21}$$

where

$$
\begin{aligned}
B_1 &= \int dJ_{01} P_J(J_{01}) \cosh(J_{01}\nabla) f(x+\gamma)|_{x=0} \\
B_2 &= \int dJ_{01} P_J(J_{01}) \sinh(J_{01}\nabla) f(x+\gamma)|_{x=0}
\end{aligned}
\tag{22}
$$

Applying s_3 to Eq. (21) will yield the three site correlation which include only perimeter spins in the cluster:

$$\langle\langle s_1 s_2 s_3 \rangle\rangle_r = B_1 \langle\langle s_1 s_2 \rangle\rangle_r + B_2 \langle\langle s_0 s_1 s_2 \rangle\rangle_r \tag{23}$$

By successive derivations we find

$$\left\langle\left\langle s_\delta^{(k)} \right\rangle\right\rangle_r = B_1 \left\langle\left\langle s_\delta^{(k-1)} \right\rangle\right\rangle_r + B_2 \left\langle\left\langle s_0 s_\delta^{(k-1)} \right\rangle\right\rangle_r \tag{24}$$

which is the correlation expression for k perimeter spins. One other possible choice for deriving correlations which include central site is to apply s_0 in Eq. (24)[9]. As seen in Ref. [9] this procedure will produce the results of BPA. By taking into account Eq. (11) we can write these correlations as

$$\left\langle\left\langle s_0 s_\delta^{(k)} \right\rangle\right\rangle_r = B_1 \left\langle\left\langle s_0 s_\delta^{(k-1)} \right\rangle\right\rangle_r + B_2 \left\langle\left\langle s_\delta^{(k-1)} \right\rangle\right\rangle_r \tag{25}$$

Thus we can get a system of linear equations by labeling the correlations;

$$
\begin{aligned}
x_k &= \left\langle\left\langle s_\delta^{(k)} \right\rangle\right\rangle_r, \quad k = 0, 1, \ldots, z; \quad x_0 = 1 \\
x_{z+k+1} &= \left\langle\left\langle s_0 s_\delta^{(k)} \right\rangle\right\rangle_r, \quad k = 0, 1, 2, \ldots, z
\end{aligned}
\tag{26}
$$

By rewriting Eq. (20) according to Eq. (26) we get

$$x_{z+k+1} = x_{k-1} T_{k-1} + x_k C_k + \sum_{n=1}^{z-2k} A_{2k+n} x_{k+n}, \quad k = 0, 1, \ldots, z \tag{27}$$

where

$$C_k = \sum_{n=0}^{k} A_{2n}, \quad T_k = \sum_{n=0}^{k} A_{2n+1}. \tag{28}$$

Similarly for Eq. (24) with Eq. (26) we have

$$x_k = B_1 x_{k-1} + B_2 x_{z+k}, \quad k = 1, 2, \ldots, z \tag{29}$$

and for Eq. (25) with Eq. (26)

$$x_{z+k+1} = B_1 x_{z+k} + B_2 x_{k-1}, \quad k = 1, 2, \ldots, z \tag{30}$$

Note that x_{-1} has to be regarded as 0 in Eq. (27).

Finally, we construct the system of linear equations based on Eqs. (27) and (29) with the coefficients given in Eqs. (16),(22) and (28). By solving this system with the condition Eq. (6) (i.e $x_1 = x_{z+1}$) we can get all representative correlations defined on the cluster and hence, we obtain better results than DA for the critical temperatures of Ising systems with coordination number z.

Another alternative choice for constructing linear equation system is forming it from Eqs. (27) for only $k = 0$, (29) and (30). The results obtained by forming equation system in this way corresponds to results in [9]. These are slightly different from results of DA. Instead of this we form our equation system from Eqs. (27) and (29). This will give better results than DA and results in [9] as seen in Section 4. This may be due to the fact that the equation system which

formed from Eqs. (27) and (29) includes smaller number of terms which have effective field than the system formed from Eqs. (27) for only $k = 0$, (29) and (30).

For completeness of the work, let us make discussions on the DA. The equation of state corresponding to DA can be obtained from Eq. (27) for $k = 0$ and by letting $x_j = m^j$ as part of Eq. (12) where m stands for $\langle\langle s_0 \rangle\rangle_r$.

$$A_0 + \sum_{n=1}^{z} A_n m^n - m = 0 \tag{31}$$

Solving (31) with coefficients given in Eq. (16) will give the magnetization within the DA. The critical temperatures can be obtained by letting $m \to 0$ in (31) and solving it for $\beta = \beta_c$[18].

4 Results and Discussion

Since the aim of this paper is to introduce an improved formulation within the EFT which is capable of calculating the multi-site correlations for any coordination number z, we give only few results in comparison with DA and EFT results. Hence, we wish to present the results of the formulation presented here only for a pure system with zero magnetic filed and for a bond diluted system (with bearing in mind that the full discussion of this problem is out of the scope of this paper) in comparison with DA and EFT results. The results of random field Ising model on three dimensional lattices can be found in our earlier work [17].

4.1 Pure System with Zero Magnetic Field

This is the simplest s-1/2 Ising system. The distribution functions are delta functions as $P_J(J_{ij}) = \delta(J_{ij} - J)$ for all i, j pairs of spins and $P_H(H_i) = \delta(H_i - H)$ where $H = 0$ for all i. Under these distributions, the coefficients of our linear equation system which are given in Eqs. (16) and (22) gets the form

$$
\begin{aligned}
A_n &= \binom{z}{n} \cosh^{z-n}(J\nabla) \sinh^n(J\nabla) f(x)|_{x=0} \\
B_1 &= \cosh(J\nabla) f(x+\gamma)|_{x=0} \\
B_2 &= \sinh(J\nabla) f(x+\gamma)|_{x=0}
\end{aligned}
\tag{32}
$$

In Eq. (32), if we write the hyperbolic functions $\cosh(J\nabla)$ and $\sinh(J\nabla)$ in terms of exponential expressions $\exp(J\nabla)$ and $\exp(-J\nabla)$, and use the binomial expansion with the differential operator technique in Eq. (7) then we can obtain more suitable forms of the coefficients A_n, B_1, B_2 as

$$
\begin{aligned}
A_n &= \frac{1}{2^z} \binom{z}{n} \sum_{r=0}^{z-n} \sum_{s=0}^{n} \binom{z-n}{r} \binom{n}{s} (-1)^s f[(z-2r-2s)J] \\
B_1 &= \frac{1}{2} [f(J+\gamma) + f(-J+\gamma)] \\
B_2 &= \frac{1}{2} [f(J+\gamma) - f(-J+\gamma)]
\end{aligned}
\tag{33}
$$

By solving the system of linear equations defined by Eqs. (27) and (29) for an arbitrary coordination number z with the coefficients given in Eqs. (28) and (33) we get the temperature dependence of the whole representative correlations defined in the system, as well as the critical temperature as a function of z by taking the limit $\gamma \to 0$ in the coefficients.

In Table 4.1, we compare the critical temperature $k_B T_c / J$ of the system obtained within the present work with those of the other methods in the literature for various coordination numbers. As seen in Table 4.1, our formulation gives the best approximated values for the numerical values of the critical temperatures when compared with MFA, EFT [9] and DA [18], which originates from the consideration of the multi-spin correlations in the system. The exact results listed in Table 4.1 are the results of high temperature series expansion method [19] which has been regarded as the exact results in the literature except the case $z = 4$ which has analytical result [20].

The improvement of this formulation is not limited with the better critical temperatures when compared with other approximations. The computability of correlations allows us to determine

some of the thermodynamic functions of the system, such as the internal energy and the specific heat.

In Fig. 1, we can see the temperature dependence of the specific heat curves which are obtained from EFT and our formulation in comparison with Monte Carlo (MC) simulation for the square lattice ($z = 4$). In MC simulation 100×100 lattice and standard Metropolis Algorithm was used. Since MC simulation gives behavior for specific heat close to real one, we can conclude from Fig. 1 that our formalism gives more accurate behavior of the specific heat than EFT. This means that formulation presented here handles two site correlations more accurate than EFT and this results in a more accurate behavior of internal energy with temperature, as well as the behavior of specific heat with temperature.
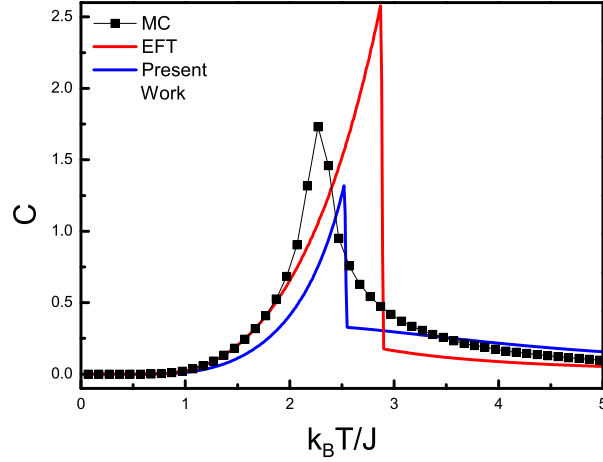

Figure 1: Variation of specific heat of square lattice with temperature for pure system under zero magnetic field. While the dotted curve shows the MC results, the red curve is EFT result and the blue one is our formulation's result.

The temperature dependencies of magnetization, internal energy and specific heat for a simple cubic lattice ($z = 6$), are shown in Fig. 3 , in comparison with DA [4] and EFT [9] as a limiting case $c = 1$ of bond diluted system.

Table 1: The critical temperatures of pure system with zero magnetic field obtained by several approximations as well as exact results and the results of the present work.

Lattice	MFA	DA [18]	EFT[9]	Present Work	Exact [19][20]
3	3.0	2.104	1.821	1.504	1.519
4	4.0	3.090	2.885	2.536	2.269
6	6.0	5.073	4.933	4.527	4.511
8	8.0	7.061	6.952	6.516	6.353
12	12.0	11.045	10.970	10.499	9.795

4.2   Bond Diluted System

Let us treat bond diluted system with zero magnetic field. The bond distribution function is given by

$$P_J\left(J_{ij}\right) = c\delta\left(J_{ij} - J\right) + (1 - c)\,\delta\left(J_{ij}\right) \tag{34}$$

and it distribute bonds randomly between lattice sites to be c percentage of bonds are closed and remaining $1 - c$ percentage of bonds are open i.e. c is the concentration of closed bonds in the lattice.

Calculating the coefficients given in Eqs. (16) and (22) by using Eq. (34) yields

$$\begin{aligned}
A_n &= \begin{pmatrix} z \\ n \end{pmatrix} [c \cosh (J\nabla) - c + 1]^{z-n} c^n \sinh^n (J\nabla) f(x)|_{x=0} \\
B_1 &= [c \cosh (J\nabla) - c + 1] f(x + \gamma)|_{x=0} \\
B_2 &= c \sinh (J\nabla) f(x + \gamma)|_{x=0}
\end{aligned} \tag{35}$$

By applying the procedure used between Eqs. (32) and (33) to Eq. (35) gives

$$\begin{aligned}
A_n &= \begin{pmatrix} z \\ n \end{pmatrix} c^n \sum_{p=0}^{z-n} \sum_{r=0}^{p} \sum_{s=0}^{n} \begin{pmatrix} z-n \\ p \end{pmatrix} \begin{pmatrix} p \\ r \end{pmatrix} \begin{pmatrix} n \\ s \end{pmatrix} \frac{c^p}{2^{n+p}} (1-c)^{z-n-p} (-1)^s f(n+p-2r-2s) \\
B_1 &= \frac{c}{2} [f(J+\gamma) + f(-J+\gamma)] + (1-c)f(\gamma) \\
B_2 &= \frac{c}{2} [f(J+\gamma) - f(-J+\gamma)]
\end{aligned} \tag{36}$$

Solving Eqs. (27) and (29) with coefficients given in Eqs. (36) and (28) gives the correlations and magnetization as a function of temperature. Again, the critical temperature of the system for a given set of Hamiltonian parameters can be obtained by letting $\gamma \to 0$. In this way the phase diagrams and the representative correlations of bond diluted s-1/2 Ising system with arbitrary coordination number z can be obtained.

The phase diagrams in $(k_B T_c / J - c)$ plane for three dimensional lattices with coordination numbers $z = 6$ (simple cubic lattice), $z = 8$ (body centered cubic lattice) and $z = 12$ (face centered cubic lattice) can be seen in Fig. 2. As seen in this figure, as the bond concentration decreases then the critical temperature values decrease gradually and fall to zero, as expected. As seen in Fig. 2 our formulation gives lower values for critical temperatures at all concentration values with respect to other two approximations. It is well known fact that for concentration values which are below a certain c^*, the system exhibits no ordered phase at all. This specific c^* value is called the critical bond concentration value. Since the formulation presented here gives lower critical temperature values at all concentration values with respect to other EFT formulations, it will give also higher critical bond concentration values. The critical bond concentration values of different lattices can be seen in Table 4.2, in comparison with the other two approximations.

The internal energy and specific heat curves as function of Hamiltonian parameters and temperature can be easily obtained within the present formulation, as well as better results for critical temperatures since the formulation is capable of calculating the multi-site correlations as well as its single site counterparts in a representative manner. This can be seen in Fig. 3 in comparison with DA and EFT. As discussed above, since the DA neglects all multi-site correlations it will give zero internal energy just above the critical temperature of the system which is physically impossible. On the other hand EFT gives more reasonable results than DA.

In Fig. 3, other than critical temperature values, clear distinction stands out between behaviors of internal energy just above the critical temperature. EFT gives energy values more close to zero for the temperatures $T > T_c$ than our formulation. Also the difference of the behaviors of energy just above the critical temperature gives rise to a difference between specific heat behaviors after T_c between EFT and formulation presented here.

The other distinction shows itself in the ground state values of magnetization and internal energy when c values get closer to the critical concentration value c^*. For these concentration values, our formalism gives lower values than EFT and DA for the ground state magnetization and internal energy. This result is expected since, while the c starting to decrease from $c = 1$, the low temperature value of magnetization gradually decreases until c reaches critical bond concentration value and our formalism gives higher critical values for bond concentration . The variation of the ground state values of this thermodynamic functions can be seen in Fig. 4 for simple cubic lattice $(z = 6)$.

As seen in Fig. 4, variation of the ground state values of magnetization and internal energy with bond concentration c for simple cubic lattice shows no significant difference for high c values, i.e. where bond diluted system is close to pure system. In contrast to this, the difference between

our formulation and the results of EFT and DA for for ground state values of magnetization and internal energy shows itself for lower c values.

Table 2: The critical bond concentration values of bond diluted system with zero magnetic field obtained by DA and EFT, as well as the results of the present work.

Lattice	DA[18]	EFT[9]	Present Work
3	0.5575	0.6623	0.7622
4	0.4284	0.4774	0.5470
6	0.2929	0.3095	0.3458
8	0.2224	0.2303	0.2520
12	0.1504	0.1528	0.1633
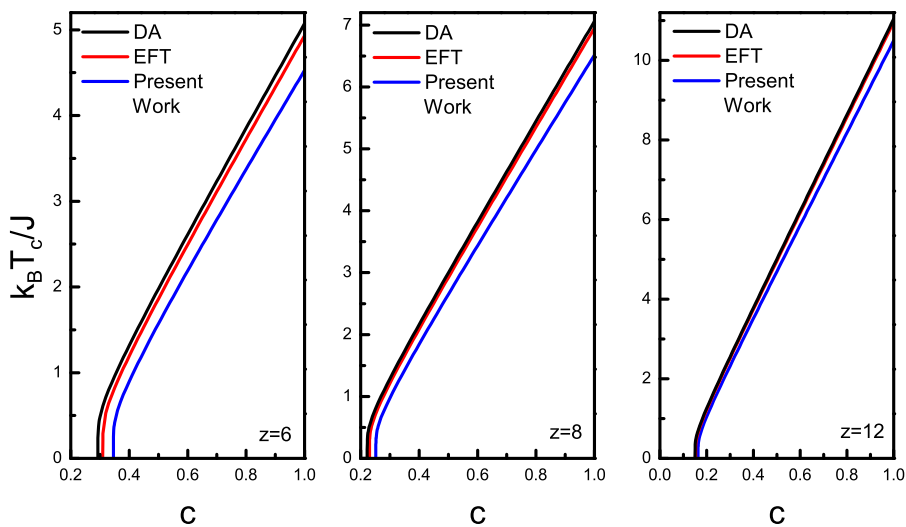
Figure 2: Variation of critical temperature for simple cubic lattice ($z = 6$), body centered cubic lattice ($z = 8$) and face centered cubic lattice ($z = 12$) with bond concentration.

5 Conclusion

In this work, we present a general formulation of s-1/2 nearest neighbor Ising system with arbitrary coordination number z. The superiority of this formulation lies under its capability of calculating correlations in a representative manner and this advantage shows itself in the results of critical temperatures and the variation of thermodynamic functions with temperature such as the magnetization and the internal energy. Formulation covers some quenched disorder effects since derivation starts with Hamiltonian (1) which include bond disorder.

Disorder effects are important in material science since disorder (like bond dilution) induce important macroscopic effects in materials. Thus it is important to obtain critical values (e.g. critical temperatures, critical bond concentrations) as well as variation of order parameter or some other thermodynamic functions (e.g. specific heat) with temperature as much as possible to the exact ones. It is a well known fact that it is impossible to obtain exact results for systems with disorder in most cases. On the other hand MC or similar simulation algorithms give accurate results for these systems but with some computational cost.
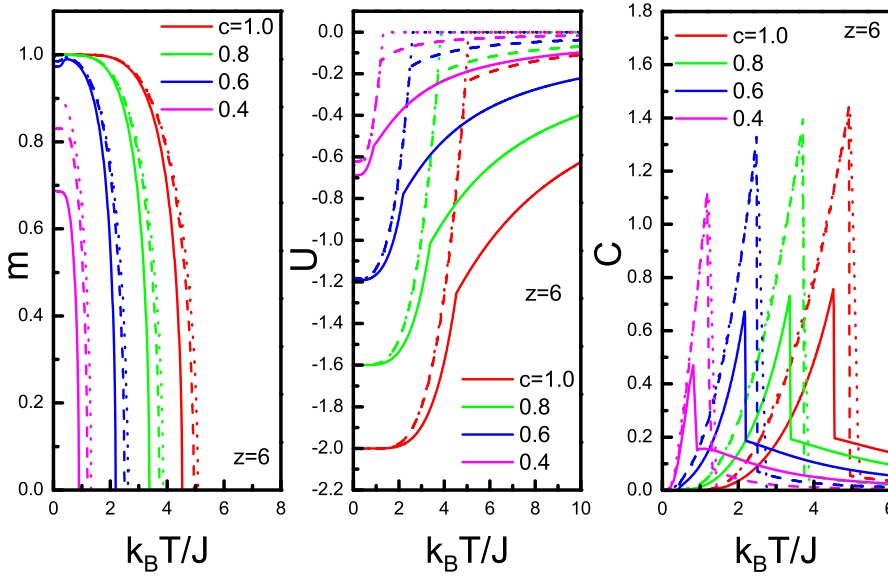
Figure 3: Variation of magnetization (m), internal energy (U) and specific heat (C) per spin of simple cubic lattice with temperature for some selected bond concentration values. The continuous lines are the results of the presented formulation, dashed lines are the result of EFT and the dotted lines are of DA.

On the other hand, as mentioned in [21],[22] some diluted antiferromagnets in uniform external magnetic field corresponds to a ferromagnet in a random external magnetic field. Then in some cases, one can obtain the behavior of more complex systems by solving s-1/2 Ising model or it's variants like random field distributed system.

This work is not the first attempt to handle the correlations which appears when expanding exact spin identities like (2). Although the most of works deal with critical behavior of spin systems within the framework of EFT, these works are based on DA which means that neglecting all multi-site correlations, there are some works handling these correlations[4], [9]. These works give results for critical temperatures as BPA. The importance of calculating these correlations are two fold. Firstly one can obtain more accurate critical values about the system and secondly one can obtain reasonable values for thermodynamic functions which are obtained from these correlations such as internal energy and the specific heat.

However, although this work is not the first attempt to handle correlations, the formulation presented here treat these correlations in a different way which give rise to more accurate results than small number of works related to it. Beyond that, we believe that it is important to obtain general formulation which covers arbitrary lattice and arbitrary Hamiltonian as long as it includes nearest neighbor interaction as a spin-spin interaction. We hope that the formulation and results obtained in this work may be beneficial form both theoretical and experimental point of view.
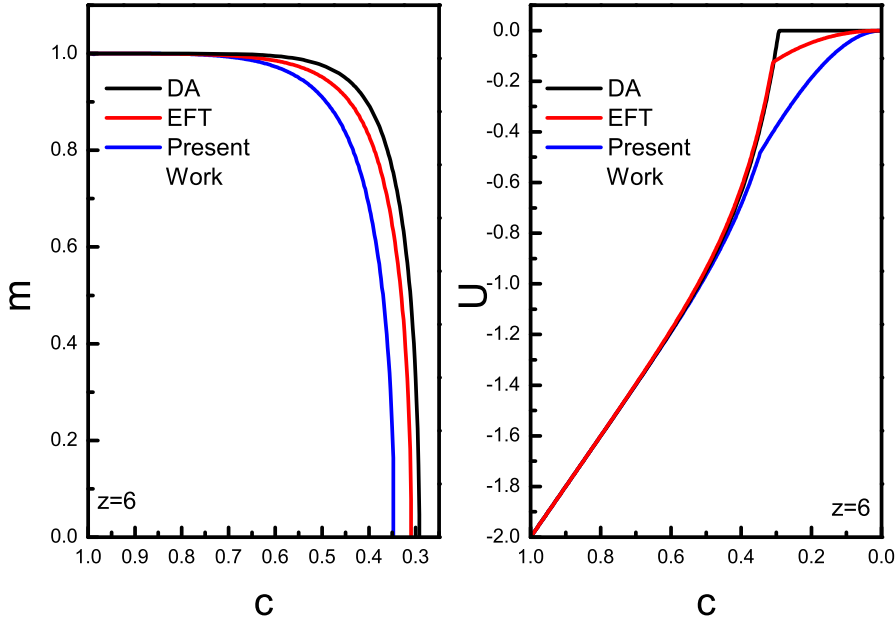
Figure 4: Variation of ground state magnetization and internal energy of simple cubic lattice ($z = 6$) with bond concentration. The calculations have been done at the temperature $T = 0.05$.

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